



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:57 AM GMT

PDB ID : 2JBM  
Title : QPRTASE STRUCTURE FROM HUMAN  
Authors : Liu, H.; Naismith, J.H.  
Deposited on : 2006-12-08  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

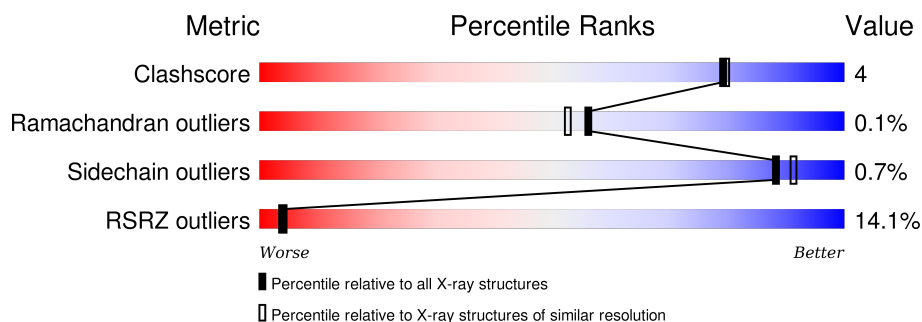
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	299	
1	B	299	
1	C	299	
1	D	299	
1	E	299	
1	F	299	
1	G	299	

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Mol	Chain	Length	Quality of chain
1	H	299	
1	I	299	
1	J	299	
1	K	299	
1	L	299	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SRT	G	401	-	-	-	X
2	SRT	H	401	-	-	-	X
2	SRT	I	401	-	-	-	X
2	SRT	L	401	-	-	-	X

## 2 Entry composition

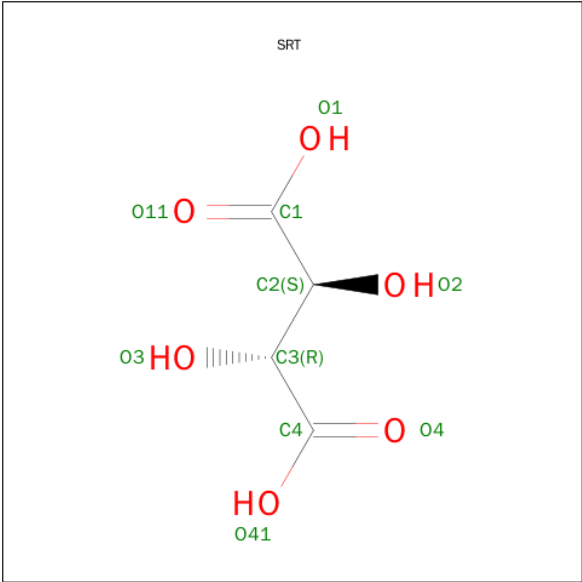
There are 3 unique types of molecules in this entry. The entry contains 28196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	1
			2109	1343	366	390	10			
1	B	289	Total	C	N	O	S	0	0	1
			2101	1338	365	389	9			
1	C	286	Total	C	N	O	S	0	0	0
			2085	1329	361	385	10			
1	D	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	E	289	Total	C	N	O	S	0	0	1
			2101	1338	365	389	9			
1	F	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	G	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	H	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	I	289	Total	C	N	O	S	0	0	1
			2101	1338	365	389	9			
1	J	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	K	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	L	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			

- Molecule 2 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		
2	C	1	Total	C	O	0	0
			10	4	6		
2	D	1	Total	C	O	0	0
			10	4	6		
2	E	1	Total	C	O	0	0
			10	4	6		
2	F	1	Total	C	O	0	0
			10	4	6		
2	G	1	Total	C	O	0	0
			10	4	6		
2	H	1	Total	C	O	0	0
			10	4	6		
2	I	1	Total	C	O	0	0
			10	4	6		
2	J	1	Total	C	O	0	0
			10	4	6		
2	K	1	Total	C	O	0	0
			10	4	6		
2	L	1	Total	C	O	0	0
			10	4	6		

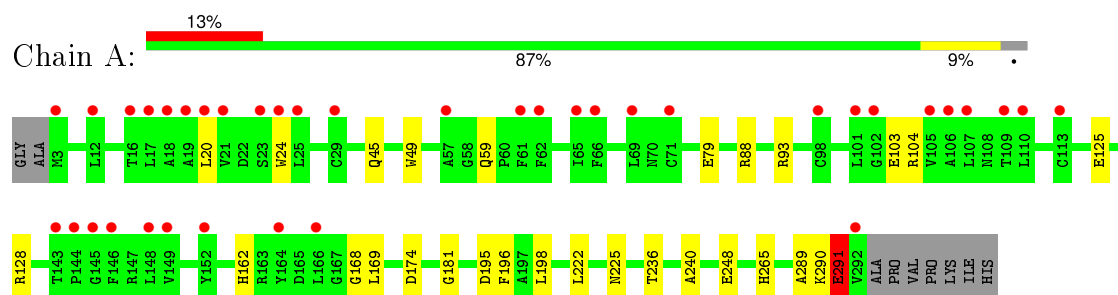
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	375	Total 375	O 375	0	0
3	B	324	Total 324	O 324	0	0
3	C	280	Total 280	O 280	0	0
3	D	292	Total 292	O 292	0	0
3	E	267	Total 267	O 267	0	0
3	F	315	Total 315	O 315	0	0
3	G	181	Total 181	O 181	0	0
3	H	127	Total 127	O 127	0	0
3	I	269	Total 269	O 269	0	0
3	J	256	Total 256	O 256	0	0
3	K	206	Total 206	O 206	0	0
3	L	148	Total 148	O 148	0	0

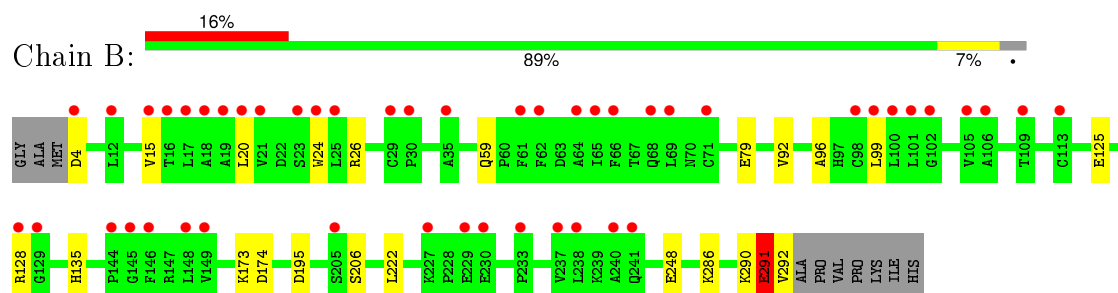
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

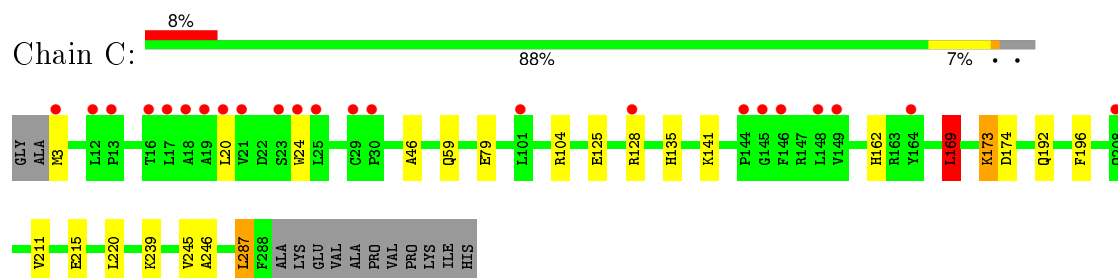
#### • Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE



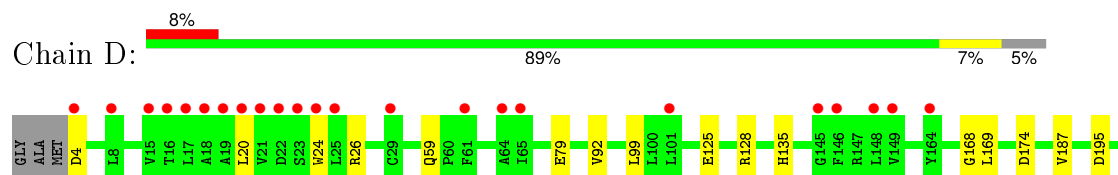
#### • Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE



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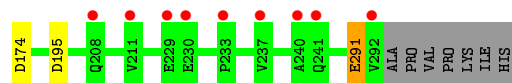
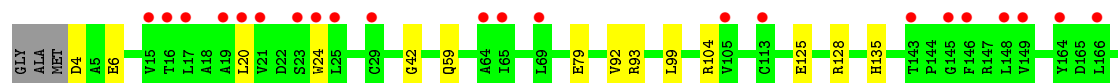
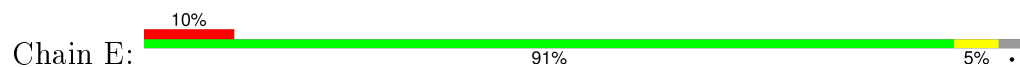


#### • Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

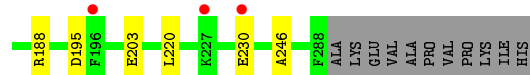
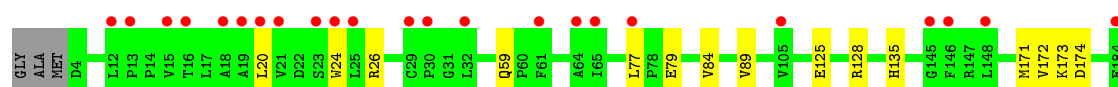
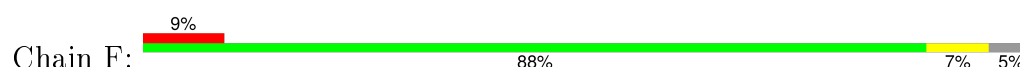




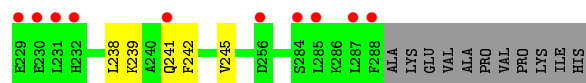
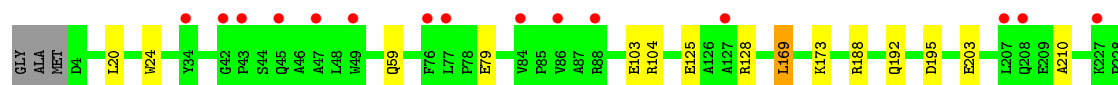
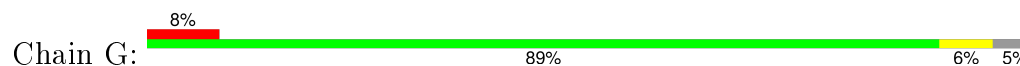
• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE



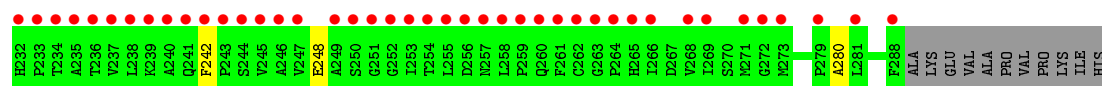
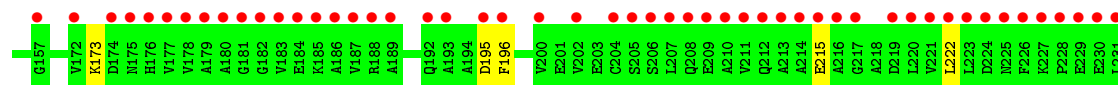
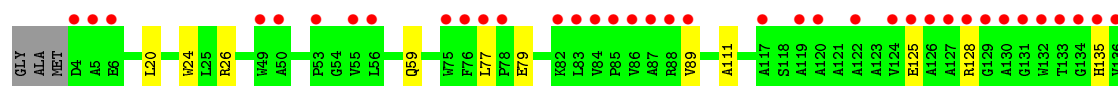
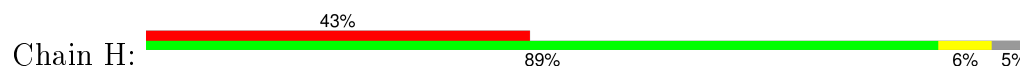
• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE



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• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.92Å 179.29Å 194.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.97 – 2.00 60.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.4 (60.97-2.00) 86.1 (60.98-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.208 0.248 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 34.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 261330 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	28196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.48 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.6514e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SRT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.65	0/2152	0.67	2/2933 (0.1%)
1	B	0.57	0/2144	0.64	1/2923 (0.0%)
1	C	0.54	0/2128	0.61	2/2901 (0.1%)
1	D	0.51	0/2120	0.60	1/2891 (0.0%)
1	E	0.54	0/2144	0.63	1/2923 (0.0%)
1	F	0.54	0/2120	0.62	1/2891 (0.0%)
1	G	0.43	0/2120	0.55	1/2891 (0.0%)
1	H	0.40	0/2120	0.52	0/2891
1	I	0.52	0/2144	0.60	1/2923 (0.0%)
1	J	0.50	0/2120	0.62	2/2891 (0.1%)
1	K	0.44	0/2120	0.53	0/2891
1	L	0.42	0/2120	0.53	0/2891
All	All	0.51	0/25552	0.60	12/34840 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	45	GLN	CA-CB-CG	8.53	132.16	113.40
1	B	174	ASP	CB-CG-OD1	7.39	124.95	118.30
1	D	174	ASP	CB-CG-OD1	6.92	124.53	118.30
1	I	174	ASP	CB-CG-OD1	6.82	124.43	118.30
1	E	174	ASP	CB-CG-OD1	6.38	124.04	118.30
1	J	45	GLN	CB-CG-CD	6.12	127.51	111.60
1	G	169	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	104	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	F	174	ASP	CB-CG-OD1	5.82	123.53	118.30
1	C	169	LEU	CA-CB-CG	5.76	128.54	115.30
1	C	174	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	104	ARG	NE-CZ-NH1	5.64	123.12	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2109	0	2128	20	3
1	B	2101	0	2119	18	0
1	C	2085	0	2104	18	0
1	D	2077	0	2095	11	0
1	E	2101	0	2119	17	0
1	F	2077	0	2095	18	0
1	G	2077	0	2095	11	0
1	H	2077	0	2095	13	0
1	I	2101	0	2119	23	3
1	J	2077	0	2095	15	0
1	K	2077	0	2095	12	0
1	L	2077	0	2095	10	0
2	A	10	0	4	1	0
2	B	10	0	4	0	0
2	C	10	0	4	2	0
2	D	10	0	4	2	0
2	E	10	0	4	0	0
2	F	10	0	4	2	0
2	G	10	0	4	1	0
2	H	10	0	4	1	0
2	I	10	0	4	0	0
2	J	10	0	4	2	0
2	K	10	0	4	0	0
2	L	10	0	4	1	0
3	A	375	0	0	11	0
3	B	324	0	0	6	0
3	C	280	0	0	7	0
3	D	292	0	0	2	0
3	E	267	0	0	10	0
3	F	315	0	0	6	0
3	G	181	0	0	2	0
3	H	127	0	0	1	0
3	I	269	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	256	0	0	7	0
3	K	206	0	0	2	0
3	L	148	0	0	5	0
All	All	28196	0	25302	178	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:HB2	3:A:2248:HOH:O	1.40	1.22
1:A:196:PHE:HB2	3:C:2187:HOH:O	1.55	1.06
1:K:128:ARG:NH1	3:K:2111:HOH:O	1.83	1.05
1:A:225:ASN:HB3	3:A:2295:HOH:O	1.58	1.01
1:C:162:HIS:CE1	3:C:2187:HOH:O	2.13	0.99
1:C:162:HIS:HE1	3:C:2187:HOH:O	1.51	0.87
1:J:229:GLU:HG3	3:J:2208:HOH:O	1.76	0.84
3:A:2249:HOH:O	1:B:286:LYS:HD2	1.77	0.83
1:L:162:HIS:HE1	3:L:2092:HOH:O	1.62	0.82
1:L:162:HIS:CE1	3:L:2092:HOH:O	2.34	0.79
1:L:180:ALA:O	1:L:185:LYS:HD3	1.83	0.79
1:E:291:GLU:HA	3:E:2265:HOH:O	1.82	0.78
1:F:230:GLU:HG3	3:F:2135:HOH:O	1.86	0.74
1:C:211:VAL:O	1:C:215:GLU:HG3	1.87	0.74
1:H:196:PHE:HB2	3:L:2092:HOH:O	1.88	0.74
1:E:291:GLU:CA	3:E:2265:HOH:O	2.37	0.73
1:I:173:LYS:HE2	3:J:2118:HOH:O	1.88	0.73
1:A:196:PHE:CB	3:C:2187:HOH:O	2.24	0.71
1:I:39:SER:O	1:I:290:LYS:NZ	2.24	0.70
1:D:195:ASP:OD1	1:E:135:HIS:ND1	2.24	0.70
1:J:46:ALA:HB2	1:J:287:LEU:HD12	1.75	0.68
1:A:181:GLY:HA2	3:A:2251:HOH:O	1.96	0.66
1:A:49:TRP:CZ3	1:A:88:ARG:HB2	2.31	0.65
1:J:77:LEU:HD12	1:J:89:VAL:HG12	1.78	0.65
1:B:4:ASP:N	3:B:2002:HOH:O	2.30	0.64
1:E:93:ARG:HD2	3:E:2127:HOH:O	1.99	0.62
1:H:196:PHE:CB	3:L:2092:HOH:O	2.45	0.62
1:D:4:ASP:N	3:D:2002:HOH:O	2.33	0.60
1:E:291:GLU:CB	3:E:2265:HOH:O	2.49	0.60
1:F:171:MET:HE3	1:F:172:VAL:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ALA:HB2	1:B:290:LYS:HD2	1.85	0.59
1:F:26:ARG:CZ	3:F:2041:HOH:O	2.51	0.58
1:J:230:GLU:HG3	3:J:2209:HOH:O	2.03	0.58
1:E:4:ASP:N	3:E:2003:HOH:O	2.36	0.58
3:A:2236:HOH:O	1:C:196:PHE:HB2	2.03	0.58
1:E:291:GLU:HG3	3:E:2265:HOH:O	2.04	0.57
1:D:135:HIS:ND1	1:E:195:ASP:OD1	2.37	0.57
1:B:195:ASP:OD1	1:F:135:HIS:ND1	2.36	0.57
1:G:210:ALA:HB1	1:G:238:LEU:HD11	1.86	0.57
1:B:20:LEU:HG	1:B:24:TRP:CZ2	2.41	0.55
1:D:20:LEU:HG	1:D:24:TRP:CZ2	2.42	0.55
1:F:26:ARG:NH1	3:F:2046:HOH:O	2.38	0.55
1:E:20:LEU:HG	1:E:24:TRP:CZ2	2.42	0.55
3:B:2053:HOH:O	1:D:26:ARG:CZ	2.54	0.54
1:E:59:GLN:HG3	1:E:79:GLU:OE1	2.06	0.54
1:A:290:LYS:O	1:A:291:GLU:HB3	2.08	0.54
1:A:103:GLU:OE2	1:B:173:LYS:NZ	2.34	0.54
1:C:104:ARG:HD3	2:D:401:SRT:O2	2.08	0.54
1:C:59:GLN:HG3	1:C:79:GLU:OE1	2.07	0.54
1:A:59:GLN:HG3	1:A:79:GLU:OE1	2.08	0.53
1:A:93:ARG:HD3	3:A:2173:HOH:O	2.08	0.53
2:D:401:SRT:H2	3:D:2172:HOH:O	2.08	0.53
1:G:103:GLU:OE2	1:H:173:LYS:NZ	2.42	0.53
1:H:215:GLU:HG2	3:H:2106:HOH:O	2.09	0.53
1:F:20:LEU:HG	1:F:24:TRP:CZ2	2.44	0.52
1:B:15:VAL:HB	3:B:2031:HOH:O	2.08	0.52
1:K:91:GLU:OE2	1:K:93:ARG:HD3	2.09	0.52
1:I:20:LEU:HG	1:I:24:TRP:CZ2	2.45	0.52
1:G:20:LEU:HG	1:G:24:TRP:CZ2	2.44	0.52
1:I:125:GLU:OE2	3:I:2147:HOH:O	2.18	0.52
1:D:59:GLN:HG3	1:D:79:GLU:OE1	2.09	0.52
1:H:26:ARG:CZ	3:J:2033:HOH:O	2.59	0.51
1:K:20:LEU:HG	1:K:24:TRP:CZ2	2.45	0.51
1:C:173:LYS:HE3	2:C:401:SRT:C1	2.40	0.51
1:I:128:ARG:CZ	3:I:2147:HOH:O	2.59	0.51
1:C:173:LYS:HE3	2:C:401:SRT:O11	2.10	0.51
1:J:20:LEU:HG	1:J:24:TRP:CZ2	2.46	0.51
2:A:401:SRT:H2	3:A:2216:HOH:O	2.09	0.51
1:H:20:LEU:HG	1:H:24:TRP:CZ2	2.45	0.51
1:H:77:LEU:HD12	1:H:89:VAL:HG22	1.93	0.51
1:A:20:LEU:HG	1:A:24:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:GLU:HG2	3:A:2371:HOH:O	2.11	0.50
1:L:20:LEU:HG	1:L:24:TRP:CZ2	2.46	0.50
1:I:125:GLU:OE1	1:I:128:ARG:NH2	2.44	0.50
1:G:241:GLN:HG2	1:G:242:PHE:CE1	2.46	0.50
1:I:104:ARG:HD3	2:J:401:SRT:O2	2.12	0.49
1:F:59:GLN:HG3	1:F:79:GLU:OE1	2.12	0.49
1:F:77:LEU:HD12	1:F:89:VAL:HG12	1.93	0.49
1:J:59:GLN:HG3	1:J:79:GLU:OE1	2.11	0.49
1:I:128:ARG:NH2	3:I:2147:HOH:O	2.45	0.49
1:B:59:GLN:HG3	1:B:79:GLU:OE1	2.12	0.49
1:D:92:VAL:HG12	1:D:99:LEU:CD2	2.42	0.49
1:J:26:ARG:CZ	3:J:2033:HOH:O	2.59	0.49
1:J:135:HIS:ND1	1:K:195:ASP:OD1	2.46	0.49
1:K:59:GLN:HG3	1:K:79:GLU:OE1	2.13	0.49
1:C:20:LEU:HG	1:C:24:TRP:CZ2	2.47	0.48
1:B:135:HIS:HD1	1:F:195:ASP:CG	2.16	0.48
1:B:286:LYS:HE2	3:B:2314:HOH:O	2.13	0.48
1:E:42:GLY:HA3	3:E:2265:HOH:O	2.14	0.48
1:I:104:ARG:HD2	2:J:401:SRT:O4	2.14	0.48
1:I:265:HIS:HD2	3:I:2239:HOH:O	1.95	0.47
1:I:173:LYS:NZ	1:J:103:GLU:OE2	2.45	0.47
1:A:45:GLN:CD	1:A:289:ALA:HB3	2.35	0.47
1:I:59:GLN:HG3	1:I:79:GLU:OE1	2.15	0.47
1:L:59:GLN:HG3	1:L:79:GLU:OE1	2.15	0.47
2:G:401:SRT:H2	3:G:2106:HOH:O	2.15	0.47
1:A:125:GLU:OE1	1:A:128:ARG:NH2	2.46	0.47
1:I:125:GLU:CD	3:I:2147:HOH:O	2.52	0.47
1:C:3:MET:HB3	3:C:2002:HOH:O	2.15	0.47
1:I:183:VAL:O	1:I:187:VAL:HG13	2.14	0.46
1:G:195:ASP:HB3	3:G:2139:HOH:O	2.16	0.46
1:G:59:GLN:HG3	1:G:79:GLU:OE1	2.15	0.46
1:G:188:ARG:O	1:G:192:GLN:HG3	2.15	0.46
1:E:6:GLU:HG3	3:E:2001:HOH:O	2.14	0.46
1:C:192:GLN:HG3	3:C:2209:HOH:O	2.15	0.46
1:K:4:ASP:N	3:K:2002:HOH:O	2.48	0.46
1:A:195:ASP:OD1	1:C:135:HIS:ND1	2.49	0.46
1:A:265:HIS:HE1	3:A:2340:HOH:O	1.98	0.45
1:C:46:ALA:HB2	1:C:287:LEU:HD12	1.97	0.45
1:L:4:ASP:HA	3:L:2001:HOH:O	2.17	0.45
1:G:125:GLU:OE1	1:G:128:ARG:NH2	2.49	0.45
2:F:401:SRT:H2	3:F:2173:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HD13	1:B:248:GLU:HG2	1.99	0.45
1:E:291:GLU:CG	3:E:2265:HOH:O	2.60	0.45
1:A:168:GLY:O	1:A:198:LEU:HD22	2.16	0.45
1:J:192:GLN:HG3	3:J:2176:HOH:O	2.16	0.45
1:K:111:ALA:HB1	1:K:280:ALA:HB1	1.99	0.45
1:B:173:LYS:HB3	1:B:173:LYS:HE3	1.82	0.44
1:I:173:LYS:HE3	1:I:173:LYS:HB3	1.67	0.44
1:G:173:LYS:HA	1:G:203:GLU:HB3	1.99	0.44
1:H:59:GLN:HG3	1:H:79:GLU:OE1	2.17	0.44
1:F:220:LEU:HG	1:F:246:ALA:HB3	1.97	0.44
1:I:92:VAL:HG12	1:I:99:LEU:CD2	2.47	0.44
1:A:225:ASN:CB	3:A:2295:HOH:O	2.35	0.44
1:G:104:ARG:HH11	2:H:401:SRT:C1	2.31	0.44
1:F:171:MET:HE3	1:F:172:VAL:H	1.83	0.44
1:C:141:LYS:HE2	3:C:2170:HOH:O	2.17	0.44
1:B:135:HIS:ND1	1:F:195:ASP:OD1	2.51	0.44
1:J:15:VAL:HB	3:J:2020:HOH:O	2.18	0.44
1:H:111:ALA:HB1	1:H:280:ALA:HB1	1.99	0.43
1:J:187:VAL:HG12	1:J:202:VAL:HG21	2.00	0.43
1:F:125:GLU:OE1	1:F:128:ARG:NH2	2.51	0.43
1:B:292:VAL:N	3:B:2320:HOH:O	2.51	0.43
1:A:222:LEU:HD13	1:A:248:GLU:HG2	1.99	0.43
1:K:44:SER:HB3	1:K:287:LEU:HD21	2.00	0.43
1:H:135:HIS:ND1	1:L:195:ASP:OD1	2.51	0.43
1:L:173:LYS:HA	1:L:203:GLU:HB3	2.01	0.43
1:C:169:LEU:O	1:C:169:LEU:HD12	2.19	0.43
1:F:84:VAL:HB	1:I:93:ARG:NH1	2.33	0.43
1:K:77:LEU:HD12	1:K:89:VAL:HG22	2.00	0.43
1:B:92:VAL:HG12	1:B:99:LEU:CD2	2.48	0.43
1:I:128:ARG:HH11	1:I:128:ARG:HG2	1.83	0.43
1:B:26:ARG:CZ	3:B:2053:HOH:O	2.66	0.43
1:H:222:LEU:HD13	1:H:248:GLU:HG2	2.01	0.43
1:H:215:GLU:HG3	1:H:242:PHE:HZ	1.83	0.43
1:E:104:ARG:HD3	2:F:401:SRT:O2	2.19	0.43
1:D:125:GLU:OE1	1:D:128:ARG:NH2	2.51	0.43
1:K:125:GLU:OE1	1:K:128:ARG:NH2	2.52	0.42
1:J:173:LYS:HA	1:J:203:GLU:HB3	2.01	0.42
1:C:239:LYS:HE2	1:C:245:VAL:O	2.19	0.42
1:H:125:GLU:OE1	1:H:128:ARG:NH2	2.53	0.42
1:I:290:LYS:O	1:I:291:GLU:CB	2.67	0.42
1:I:174:ASP:HB2	3:I:2182:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:VAL:HG12	1:D:202:VAL:HG21	2.03	0.41
1:F:173:LYS:HA	1:F:203:GLU:HB3	2.02	0.41
1:L:163:ARG:HE	2:L:401:SRT:C4	2.34	0.41
1:E:93:ARG:NH2	3:E:2126:HOH:O	2.53	0.41
1:A:162:HIS:CE1	3:A:2236:HOH:O	2.73	0.41
1:F:77:LEU:HG	3:I:2117:HOH:O	2.19	0.41
1:K:75:TRP:CE3	1:K:90:ALA:HB2	2.56	0.41
1:E:92:VAL:HG12	1:E:99:LEU:CD2	2.50	0.41
1:D:168:GLY:O	1:D:198:LEU:HD22	2.20	0.41
1:I:239:LYS:HE3	1:I:247:VAL:HG23	2.03	0.41
1:G:239:LYS:HE2	1:G:245:VAL:O	2.20	0.41
1:C:125:GLU:OE1	1:C:128:ARG:NH2	2.53	0.41
1:F:195:ASP:HB3	3:F:2232:HOH:O	2.21	0.41
1:I:222:LEU:HD13	1:I:248:GLU:HG2	2.02	0.41
1:D:222:LEU:HD13	1:D:248:GLU:HG2	2.03	0.41
1:J:48:LEU:HD23	1:J:89:VAL:HG23	2.03	0.41
1:J:173:LYS:HE3	1:J:173:LYS:HB2	1.94	0.41
1:C:220:LEU:HG	1:C:246:ALA:HB3	2.03	0.41
1:E:125:GLU:OE1	1:E:128:ARG:NH2	2.52	0.40
1:L:132:TRP:HB2	1:L:262:CYS:HB3	2.03	0.40
1:F:188:ARG:NH2	3:F:2219:HOH:O	2.52	0.40
1:B:125:GLU:OE1	1:B:128:ARG:NH2	2.55	0.40
1:I:290:LYS:NZ	3:I:2263:HOH:O	2.43	0.40
1:B:290:LYS:O	1:B:291:GLU:HB2	2.21	0.40
1:K:21:VAL:HG22	1:K:65:ILE:HG13	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ALA:CB	1:I:128:ARG:NH1[4_466]	1.25	0.95
1:A:236:THR:CG2	1:I:125:GLU:OE2[4_466]	1.67	0.53
1:A:240:ALA:CA	1:I:128:ARG:NH1[4_466]	1.84	0.36

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/299 (96%)	284 (99%)	3 (1%)	1 (0%)	46	41
1	B	287/299 (96%)	281 (98%)	5 (2%)	1 (0%)	46	41
1	C	284/299 (95%)	281 (99%)	3 (1%)	0	100	100
1	D	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
1	E	287/299 (96%)	281 (98%)	5 (2%)	1 (0%)	46	41
1	F	283/299 (95%)	281 (99%)	2 (1%)	0	100	100
1	G	283/299 (95%)	279 (99%)	4 (1%)	0	100	100
1	H	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
1	I	287/299 (96%)	282 (98%)	4 (1%)	1 (0%)	46	41
1	J	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
1	K	283/299 (95%)	279 (99%)	4 (1%)	0	100	100
1	L	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
All	All	3414/3588 (95%)	3368 (99%)	42 (1%)	4 (0%)	56	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	GLU
1	B	291	GLU
1	E	291	GLU
1	I	291	GLU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/219 (97%)	210 (99%)	2 (1%)	84	88
1	B	211/219 (96%)	209 (99%)	2 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	210/219 (96%)	207 (99%)	3 (1%)	74	77
1	D	209/219 (95%)	208 (100%)	1 (0%)	92	94
1	E	211/219 (96%)	211 (100%)	0	100	100
1	F	209/219 (95%)	209 (100%)	0	100	100
1	G	209/219 (95%)	208 (100%)	1 (0%)	92	94
1	H	209/219 (95%)	208 (100%)	1 (0%)	92	94
1	I	211/219 (96%)	209 (99%)	2 (1%)	84	88
1	J	209/219 (95%)	207 (99%)	2 (1%)	82	85
1	K	209/219 (95%)	208 (100%)	1 (0%)	92	94
1	L	209/219 (95%)	207 (99%)	2 (1%)	82	85
All	All	2518/2628 (96%)	2501 (99%)	17 (1%)	88	91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	A	291	GLU
1	B	206	SER
1	B	291	GLU
1	C	169	LEU
1	C	173	LYS
1	C	287	LEU
1	D	169	LEU
1	G	169	LEU
1	H	195	ASP
1	I	184	GLU
1	I	244	SER
1	J	45	GLN
1	J	241	GLN
1	K	287	LEU
1	L	188	ARG
1	L	287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	HIS

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Mol	Chain	Res	Type
1	C	162	HIS
1	D	192	GLN
1	E	265	HIS
1	I	265	HIS
1	I	276	GLN
1	J	265	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SRT	A	401	-	3,9,9	0.22	0	6,12,12	2.38	2 (33%)
2	SRT	B	401	-	3,9,9	0.13	0	6,12,12	1.26	1 (16%)
2	SRT	C	401	-	3,9,9	0.18	0	6,12,12	1.79	1 (16%)
2	SRT	D	401	-	3,9,9	0.41	0	6,12,12	2.16	2 (33%)
2	SRT	E	401	-	3,9,9	0.34	0	6,12,12	1.25	1 (16%)
2	SRT	F	401	-	3,9,9	0.23	0	6,12,12	2.92	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SRT	G	401	-	3,9,9	0.20	0	6,12,12	1.19	0
2	SRT	H	401	-	3,9,9	0.24	0	6,12,12	1.20	0
2	SRT	I	401	-	3,9,9	0.26	0	6,12,12	1.45	1 (16%)
2	SRT	J	401	-	3,9,9	0.45	0	6,12,12	2.98	3 (50%)
2	SRT	K	401	-	3,9,9	0.41	0	6,12,12	1.57	2 (33%)
2	SRT	L	401	-	3,9,9	0.63	0	6,12,12	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SRT	A	401	-	-	0/4/12/12	0/0/0/0
2	SRT	B	401	-	-	0/4/12/12	0/0/0/0
2	SRT	C	401	-	-	0/4/12/12	0/0/0/0
2	SRT	D	401	-	-	0/4/12/12	0/0/0/0
2	SRT	E	401	-	-	0/4/12/12	0/0/0/0
2	SRT	F	401	-	-	0/4/12/12	0/0/0/0
2	SRT	G	401	-	-	0/4/12/12	0/0/0/0
2	SRT	H	401	-	-	0/4/12/12	0/0/0/0
2	SRT	I	401	-	-	0/4/12/12	0/0/0/0
2	SRT	J	401	-	-	0/4/12/12	0/0/0/0
2	SRT	K	401	-	-	0/4/12/12	0/0/0/0
2	SRT	L	401	-	-	0/4/12/12	0/0/0/0

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	SRT	O3-C3-C2	-6.06	91.52	108.61
2	F	401	SRT	O3-C3-C2	-4.95	94.66	108.61
2	D	401	SRT	O3-C3-C2	-4.53	95.85	108.61
2	A	401	SRT	O3-C3-C2	-4.20	96.77	108.61
2	C	401	SRT	O3-C3-C2	-3.53	98.68	108.61
2	I	401	SRT	O3-C3-C2	-2.95	100.29	108.61
2	B	401	SRT	O3-C3-C2	-2.38	101.90	108.61
2	E	401	SRT	C1-C2-C3	-2.32	108.59	113.35
2	K	401	SRT	O3-C3-C2	-2.26	102.25	108.61
2	D	401	SRT	O2-C2-C3	2.03	114.34	108.61
2	K	401	SRT	O2-C2-C3	2.25	114.95	108.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	SRT	O2-C2-C3	2.40	115.39	108.61
2	J	401	SRT	O2-C2-C1	2.59	117.75	111.21
2	A	401	SRT	O2-C2-C3	2.92	116.84	108.61
2	F	401	SRT	O2-C2-C1	2.94	118.64	111.21
2	F	401	SRT	O2-C2-C3	3.90	119.60	108.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SRT	1	0
2	C	401	SRT	2	0
2	D	401	SRT	2	0
2	F	401	SRT	2	0
2	G	401	SRT	1	0
2	H	401	SRT	1	0
2	J	401	SRT	2	0
2	L	401	SRT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	290/299 (96%)	0.96	38 (13%) 5 5	2, 7, 13, 31	0
1	B	289/299 (96%)	0.86	48 (16%) 2 3	2, 7, 13, 21	0
1	C	286/299 (95%)	0.54	23 (8%) 15 16	2, 7, 13, 28	0
1	D	285/299 (95%)	0.56	24 (8%) 14 14	2, 7, 12, 21	0
1	E	289/299 (96%)	0.72	31 (10%) 8 8	2, 7, 13, 25	0
1	F	285/299 (95%)	0.57	26 (9%) 11 12	2, 7, 12, 21	0
1	G	285/299 (95%)	0.75	25 (8%) 12 13	2, 7, 12, 21	0
1	H	285/299 (95%)	1.94	130 (45%) 0 1	2, 7, 12, 21	0
1	I	289/299 (96%)	0.31	7 (2%) 62 63	2, 7, 13, 25	0
1	J	285/299 (95%)	0.46	19 (6%) 21 22	2, 7, 12, 21	0
1	K	285/299 (95%)	0.38	17 (5%) 25 27	2, 7, 12, 21	0
1	L	285/299 (95%)	1.39	96 (33%) 0 1	2, 7, 12, 21	0
All	All	3438/3588 (95%)	0.79	484 (14%) 4 4	2, 7, 13, 31	0

All (484) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	292	VAL	13.3
1	A	292	VAL	12.5
1	H	207	LEU	9.0
1	E	292	VAL	8.8
1	H	231	LEU	7.5
1	H	134	GLY	7.1
1	H	4	ASP	6.9
1	H	262	CYS	6.8
1	H	213	ALA	6.3
1	H	238	LEU	6.1
1	L	231	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	H	240	ALA	5.5
1	H	131	GLY	5.5
1	H	180	ALA	5.4
1	H	128	ARG	5.3
1	H	206	SER	5.3
1	H	211	VAL	5.2
1	H	230	GLU	5.2
1	H	233	PRO	5.2
1	L	242	PHE	5.2
1	H	135	HIS	5.2
1	H	208	GLN	5.2
1	L	188	ARG	5.2
1	L	208	GLN	5.0
1	H	263	GLY	5.0
1	L	252	GLY	4.9
1	H	196	PHE	4.9
1	H	226	PHE	4.9
1	L	238	LEU	4.8
1	H	132	TRP	4.8
1	H	133	THR	4.8
1	L	132	TRP	4.8
1	L	243	PRO	4.8
1	K	128	ARG	4.8
1	L	131	GLY	4.8
1	H	235	ALA	4.7
1	H	265	HIS	4.7
1	G	49	TRP	4.7
1	H	214	ALA	4.7
1	L	240	ALA	4.7
1	H	184	GLU	4.7
1	H	205	SER	4.6
1	H	237	VAL	4.6
1	H	210	ALA	4.6
1	H	255	LEU	4.6
1	L	227	LYS	4.5
1	A	19	ALA	4.4
1	L	266	ILE	4.4
1	H	244	SER	4.4
1	H	234	THR	4.4
1	H	266	ILE	4.4
1	H	124	VAL	4.4
1	H	232	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	181	GLY	4.3
1	L	207	LEU	4.3
1	L	196	PHE	4.2
1	H	229	GLU	4.2
1	H	227	LYS	4.2
1	L	130	ALA	4.2
1	B	19	ALA	4.2
1	H	129	GLY	4.2
1	L	260	GLN	4.2
1	H	236	THR	4.1
1	H	86	VAL	4.1
1	H	126	ALA	4.1
1	L	126	ALA	4.1
1	G	288	PHE	4.1
1	H	269	ILE	4.0
1	L	261	PHE	4.0
1	H	242	PHE	4.0
1	L	235	ALA	4.0
1	H	261	PHE	4.0
1	H	82	LYS	4.0
1	H	258	LEU	3.9
1	H	268	VAL	3.9
1	L	195	ASP	3.9
1	G	227	LYS	3.8
1	L	206	SER	3.8
1	E	229	GLU	3.8
1	H	186	ALA	3.8
1	H	257	ASN	3.8
1	E	230	GLU	3.7
1	H	246	ALA	3.7
1	H	136	VAL	3.7
1	L	269	ILE	3.7
1	B	24	TRP	3.6
1	H	228	PRO	3.6
1	C	19	ALA	3.6
1	A	25	LEU	3.6
1	A	20	LEU	3.6
1	L	229	GLU	3.6
1	L	127	ALA	3.6
1	H	172	VAL	3.5
1	H	157	GLY	3.5
1	H	221	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	182	GLY	3.5
1	C	20	LEU	3.5
1	H	264	PRO	3.5
1	L	237	VAL	3.5
1	B	17	LEU	3.5
1	G	231	LEU	3.5
1	C	18	ALA	3.5
1	H	188	ARG	3.5
1	L	180	ALA	3.5
1	H	239	LYS	3.5
1	C	21	VAL	3.5
1	L	183	VAL	3.5
1	C	3	MET	3.5
1	H	87	ALA	3.5
1	H	250	SER	3.4
1	H	212	GLN	3.4
1	B	145	GLY	3.4
1	D	24	TRP	3.4
1	H	5	ALA	3.4
1	H	179	ALA	3.4
1	H	53	PRO	3.4
1	H	217	GLY	3.4
1	H	216	ALA	3.4
1	H	247	VAL	3.4
1	L	258	LEU	3.4
1	L	134	GLY	3.4
1	E	16	THR	3.3
1	H	84	VAL	3.3
1	I	128	ARG	3.3
1	F	196	PHE	3.3
1	L	226	PHE	3.3
1	D	19	ALA	3.3
1	E	21	VAL	3.3
1	L	245	VAL	3.3
1	J	252	GLY	3.3
1	H	223	LEU	3.3
1	L	230	GLU	3.3
1	A	21	VAL	3.3
1	L	136	VAL	3.3
1	L	232	HIS	3.3
1	H	127	ALA	3.3
1	L	214	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	265	HIS	3.3
1	D	20	LEU	3.3
1	H	49	TRP	3.3
1	H	251	GLY	3.2
1	L	6	GLU	3.2
1	L	247	VAL	3.2
1	H	77	LEU	3.2
1	G	86	VAL	3.2
1	L	225	ASN	3.2
1	L	233	PRO	3.2
1	L	211	VAL	3.2
1	H	224	ASP	3.2
1	L	262	CYS	3.2
1	G	229	GLU	3.2
1	A	106	ALA	3.2
1	B	65	ILE	3.2
1	L	128	ARG	3.2
1	H	187	VAL	3.2
1	H	195	ASP	3.1
1	H	252	GLY	3.1
1	L	251	GLY	3.1
1	I	256	ASP	3.1
1	L	204	CYS	3.1
1	H	83	LEU	3.1
1	C	145	GLY	3.1
1	F	19	ALA	3.1
1	L	4	ASP	3.1
1	L	244	SER	3.1
1	D	15	VAL	3.1
1	L	217	GLY	3.1
1	B	20	LEU	3.1
1	B	64	ALA	3.1
1	E	237	VAL	3.1
1	K	211	VAL	3.1
1	B	146	PHE	3.1
1	G	76	PHE	3.1
1	L	181	GLY	3.1
1	B	106	ALA	3.0
1	L	133	THR	3.0
1	B	18	ALA	3.0
1	H	222	LEU	3.0
1	B	16	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	146	PHE	3.0
1	L	129	GLY	3.0
1	H	183	VAL	3.0
1	L	234	THR	3.0
1	B	25	LEU	3.0
1	C	25	LEU	3.0
1	D	148	LEU	3.0
1	D	146	PHE	3.0
1	F	18	ALA	3.0
1	L	246	ALA	3.0
1	G	230	GLU	3.0
1	B	4	ASP	3.0
1	H	174	ASP	3.0
1	H	256	ASP	3.0
1	G	241	GLN	3.0
1	B	128	ARG	2.9
1	D	29	CYS	2.9
1	D	17	LEU	2.9
1	H	200	VAL	2.9
1	H	260	GLN	2.9
1	L	191	ARG	2.9
1	L	213	ALA	2.9
1	E	233	PRO	2.9
1	L	49	TRP	2.9
1	C	148	LEU	2.9
1	G	207	LEU	2.9
1	A	105	VAL	2.9
1	L	249	ALA	2.9
1	A	113	CYS	2.9
1	B	69	LEU	2.9
1	H	185	LYS	2.9
1	L	239	LYS	2.9
1	L	135	HIS	2.9
1	L	205	SER	2.9
1	L	77	LEU	2.9
1	A	24	TRP	2.9
1	B	29	CYS	2.9
1	B	61	PHE	2.9
1	G	256	ASP	2.9
1	J	227	LYS	2.9
1	L	86	VAL	2.9
1	H	193	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	24	TRP	2.9
1	L	264	PRO	2.9
1	F	230	GLU	2.9
1	L	182	GLY	2.8
1	H	125	GLU	2.8
1	H	273	MET	2.8
1	L	256	ASP	2.8
1	H	241	GLN	2.8
1	D	16	THR	2.8
1	E	146	PHE	2.8
1	J	4	ASP	2.8
1	H	78	PRO	2.8
1	E	19	ALA	2.8
1	H	120	ALA	2.8
1	L	210	ALA	2.8
1	B	101	LEU	2.8
1	G	287	LEU	2.8
1	A	149	VAL	2.8
1	H	209	GLU	2.8
1	J	243	PRO	2.8
1	A	18	ALA	2.8
1	H	177	VAL	2.8
1	K	208	GLN	2.8
1	H	243	PRO	2.8
1	G	47	ALA	2.8
1	L	83	LEU	2.8
1	H	189	ALA	2.7
1	D	65	ILE	2.7
1	E	20	LEU	2.7
1	F	21	VAL	2.7
1	D	23	SER	2.7
1	H	88	ARG	2.7
1	H	288	PHE	2.7
1	L	218	ALA	2.7
1	A	148	LEU	2.7
1	F	24	TRP	2.7
1	L	241	GLN	2.7
1	B	230	GLU	2.7
1	F	16	THR	2.7
1	J	230	GLU	2.7
1	H	225	ASN	2.7
1	D	18	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	212	GLN	2.7
1	D	61	PHE	2.7
1	H	271	MET	2.7
1	F	148	LEU	2.7
1	C	208	GLN	2.6
1	G	77	LEU	2.6
1	H	220	LEU	2.6
1	I	125	GLU	2.6
1	C	144	PRO	2.6
1	H	272	GLY	2.6
1	A	101	LEU	2.6
1	B	21	VAL	2.6
1	C	16	THR	2.6
1	H	178	VAL	2.6
1	H	50	ALA	2.6
1	G	208	GLN	2.6
1	D	164	TYR	2.6
1	H	192	GLN	2.6
1	L	84	VAL	2.6
1	J	131	GLY	2.6
1	F	20	LEU	2.6
1	L	220	LEU	2.6
1	F	65	ILE	2.6
1	H	119	ALA	2.6
1	L	5	ALA	2.6
1	D	149	VAL	2.6
1	A	3	MET	2.6
1	E	164	TYR	2.6
1	E	17	LEU	2.6
1	E	65	ILE	2.6
1	H	253	ILE	2.6
1	L	177	VAL	2.6
1	A	164	TYR	2.5
1	B	23	SER	2.5
1	G	284	SER	2.5
1	K	230	GLU	2.5
1	L	287	LEU	2.5
1	H	219	ASP	2.5
1	H	215	GLU	2.5
1	K	243	PRO	2.5
1	G	88	ARG	2.5
1	A	71	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	215	GLU	2.5
1	C	23	SER	2.5
1	A	102	GLY	2.5
1	C	128	ARG	2.5
1	E	240	ALA	2.5
1	H	122	ALA	2.5
1	E	148	LEU	2.5
1	E	24	TRP	2.5
1	H	259	PRO	2.5
1	L	209	GLU	2.5
1	A	57	ALA	2.5
1	H	76	PHE	2.5
1	B	98	CYS	2.5
1	C	30	PRO	2.5
1	E	113	CYS	2.5
1	L	221	VAL	2.5
1	C	146	PHE	2.5
1	B	30	PRO	2.5
1	I	4	ASP	2.5
1	E	15	VAL	2.5
1	H	202	VAL	2.5
1	J	262	CYS	2.5
1	J	236	THR	2.5
1	L	254	THR	2.5
1	C	164	TYR	2.4
1	F	146	PHE	2.4
1	A	17	LEU	2.4
1	B	149	VAL	2.4
1	H	204	CYS	2.4
1	H	117	ALA	2.4
1	B	148	LEU	2.4
1	C	12	LEU	2.4
1	J	237	VAL	2.4
1	L	15	VAL	2.4
1	B	229	GLU	2.4
1	H	130	ALA	2.4
1	A	29	CYS	2.4
1	H	176	HIS	2.4
1	B	238	LEU	2.4
1	H	56	LEU	2.4
1	D	21	VAL	2.4
1	F	30	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	279	PRO	2.4
1	B	71	CYS	2.4
1	C	29	CYS	2.4
1	C	17	LEU	2.4
1	G	285	LEU	2.4
1	F	13	PRO	2.4
1	L	253	ILE	2.4
1	I	208	GLN	2.4
1	B	100	LEU	2.4
1	C	101	LEU	2.4
1	D	145	GLY	2.4
1	H	6	GLU	2.4
1	I	229	GLU	2.4
1	E	208	GLN	2.3
1	K	252	GLY	2.3
1	D	25	LEU	2.3
1	E	25	LEU	2.3
1	A	66	PHE	2.3
1	B	233	PRO	2.3
1	G	45	GLN	2.3
1	C	149	VAL	2.3
1	K	241	GLN	2.3
1	L	76	PHE	2.3
1	B	240	ALA	2.3
1	E	64	ALA	2.3
1	H	245	VAL	2.3
1	F	25	LEU	2.3
1	A	61	PHE	2.3
1	J	261	PHE	2.3
1	L	186	ALA	2.3
1	E	211	VAL	2.3
1	A	109	THR	2.3
1	D	101	LEU	2.3
1	L	222	LEU	2.3
1	L	174	ASP	2.3
1	A	145	GLY	2.3
1	B	205	SER	2.3
1	E	105	VAL	2.3
1	H	55	VAL	2.3
1	J	253	ILE	2.3
1	L	228	PRO	2.3
1	J	128	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	69	LEU	2.3
1	E	23	SER	2.2
1	E	145	GLY	2.2
1	E	149	VAL	2.2
1	F	15	VAL	2.2
1	F	184	GLU	2.2
1	H	89	VAL	2.2
1	H	254	THR	2.2
1	D	208	GLN	2.2
1	C	13	PRO	2.2
1	E	143	THR	2.2
1	L	87	ALA	2.2
1	F	105	VAL	2.2
1	B	129	GLY	2.2
1	F	227	LYS	2.2
1	L	161	SER	2.2
1	L	263	GLY	2.2
1	D	64	ALA	2.2
1	F	64	ALA	2.2
1	F	29	CYS	2.2
1	D	8	LEU	2.2
1	H	85	PRO	2.2
1	B	66	PHE	2.2
1	E	29	CYS	2.2
1	A	110	LEU	2.2
1	H	75	TRP	2.2
1	A	143	THR	2.2
1	F	23	SER	2.2
1	L	115	GLY	2.2
1	D	22	ASP	2.2
1	G	34	TYR	2.2
1	J	229	GLU	2.2
1	B	105	VAL	2.2
1	H	249	ALA	2.2
1	A	107	LEU	2.1
1	F	12	LEU	2.1
1	K	231	LEU	2.1
1	F	145	GLY	2.1
1	B	62	PHE	2.1
1	F	61	PHE	2.1
1	L	257	ASN	2.1
1	G	127	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	43	PRO	2.1
1	K	236	THR	2.1
1	J	242	PHE	2.1
1	L	179	ALA	2.1
1	B	15	VAL	2.1
1	G	84	VAL	2.1
1	J	233	PRO	2.1
1	A	16	THR	2.1
1	A	166	LEU	2.1
1	F	77	LEU	2.1
1	K	255	LEU	2.1
1	B	241	GLN	2.1
1	L	125	GLU	2.1
1	A	144	PRO	2.1
1	L	190	ALA	2.1
1	G	232	HIS	2.1
1	J	184	GLU	2.1
1	B	99	LEU	2.1
1	B	35	ALA	2.1
1	G	42	GLY	2.1
1	H	175	ASN	2.1
1	J	226	PHE	2.1
1	B	237	VAL	2.1
1	J	260	GLN	2.1
1	D	4	ASP	2.1
1	K	256	ASP	2.1
1	L	224	ASP	2.1
1	H	281	LEU	2.1
1	K	88	ARG	2.1
1	E	241	GLN	2.1
1	A	62	PHE	2.1
1	K	237	VAL	2.1
1	L	215	GLU	2.0
1	B	144	PRO	2.0
1	B	227	LYS	2.0
1	A	12	LEU	2.0
1	B	68	GLN	2.0
1	E	69	LEU	2.0
1	L	223	LEU	2.0
1	B	102	GLY	2.0
1	K	205	SER	2.0
1	K	4	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	109	THR	2.0
1	A	98	CYS	2.0
1	B	113	CYS	2.0
1	B	12	LEU	2.0
1	E	166	LEU	2.0
1	F	32	LEU	2.0
1	J	238	LEU	2.0
1	K	45	GLN	2.0
1	A	152	TYR	2.0
1	A	23	SER	2.0
1	A	65	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SRT	G	401	10/10	0.85	0.19	4.66	19,22,23,25	0
2	SRT	L	401	10/10	0.85	0.28	3.47	19,22,25,25	0
2	SRT	H	401	10/10	0.78	0.34	3.42	16,18,21,22	0
2	SRT	I	401	10/10	0.78	0.20	3.39	16,22,26,27	0
2	SRT	E	401	10/10	0.88	0.18	0.83	10,16,19,24	0
2	SRT	A	401	10/10	0.90	0.19	0.49	15,19,22,22	0
2	SRT	K	401	10/10	0.88	0.14	0.40	12,16,17,17	0
2	SRT	J	401	10/10	0.92	0.13	0.34	7,11,13,13	0
2	SRT	B	401	10/10	0.84	0.17	0.33	16,20,24,24	0
2	SRT	D	401	10/10	0.84	0.15	-0.11	16,20,20,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SRT	C	401	10/10	0.92	0.15	-0.32	16,19,23,24	0
2	SRT	F	401	10/10	0.91	0.13	-0.61	8,15,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.